

#### A Computational Design Study of Self-healing Creep Resistant Steels

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# A Computational Design Study of Self-healing Creep Resistant Steels

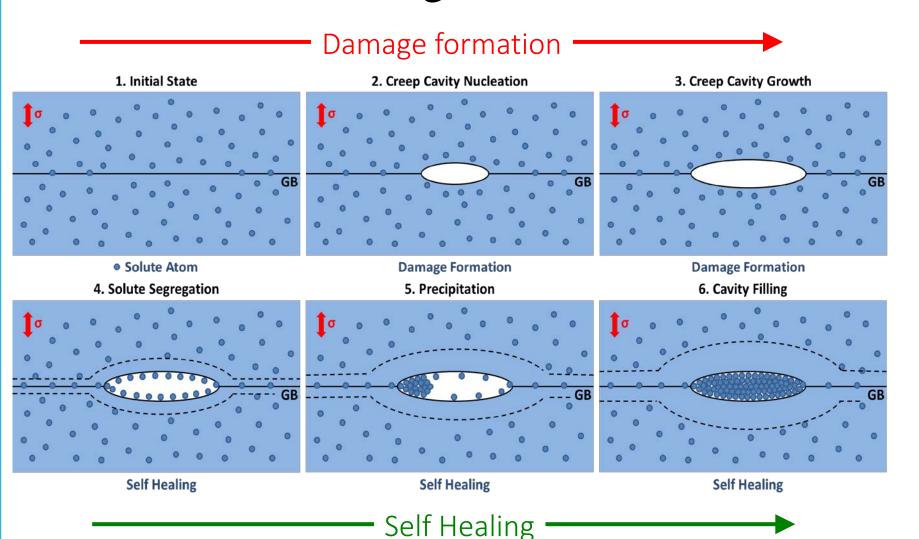
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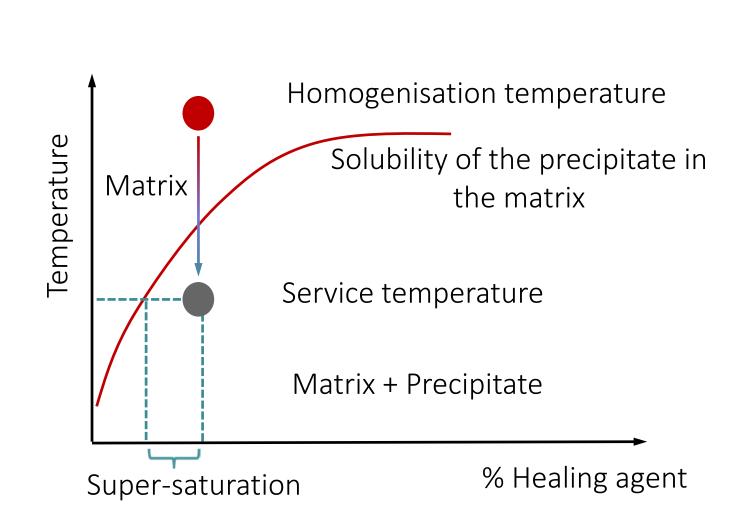
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# Background

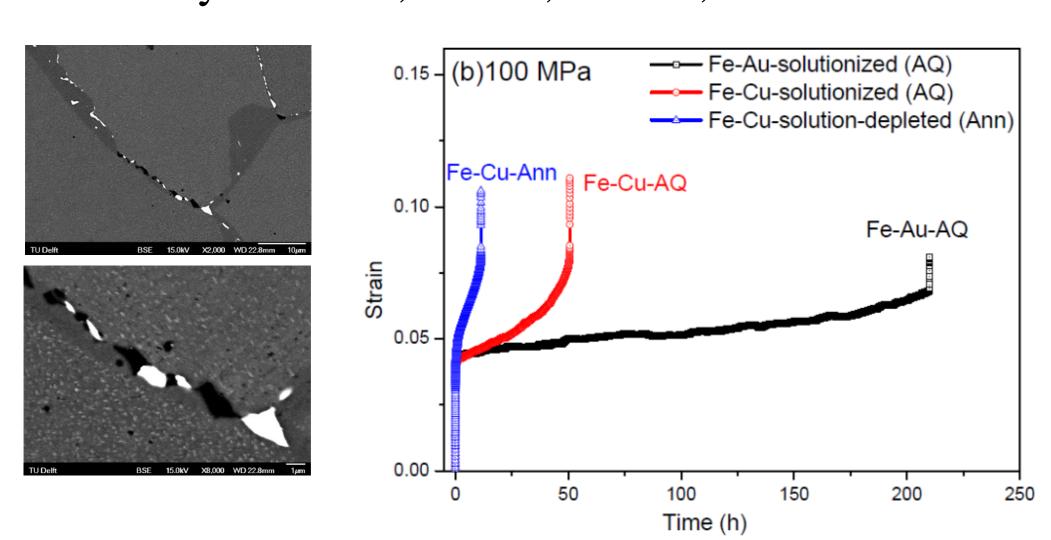
Self-healing behaviour [1]



Precipitation-based self-healing alloy



Model alloys: Fe-Cu, Fe-Au, Fe-Mo, Fe-W

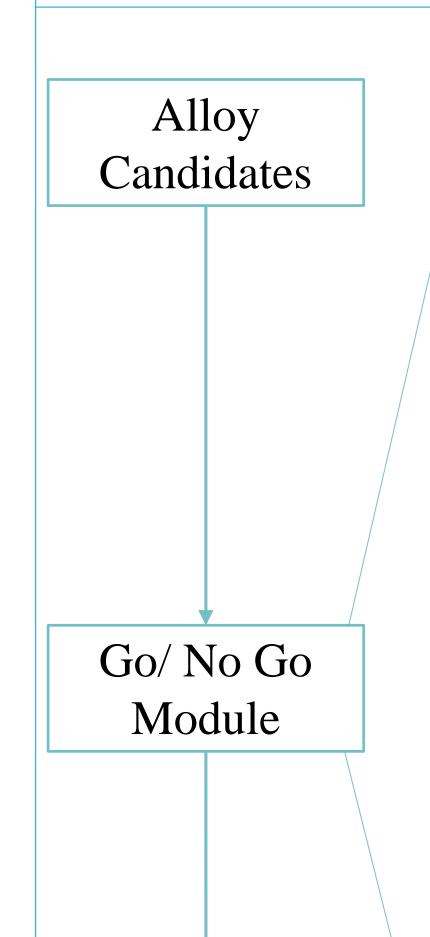


Au-riched precipitation and the enhanced creep lifetime [1]

1100

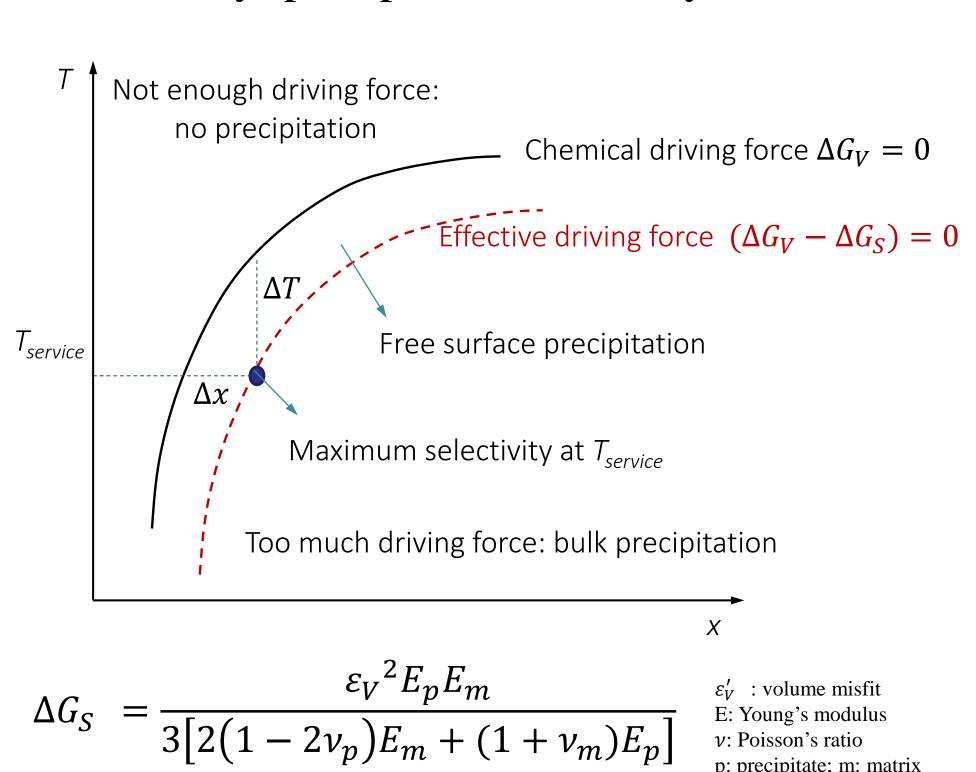
• Aim: a multi-elemental, self-healable, creep resistant ferrous system with adequate mechanical properties for elevated temperature use.

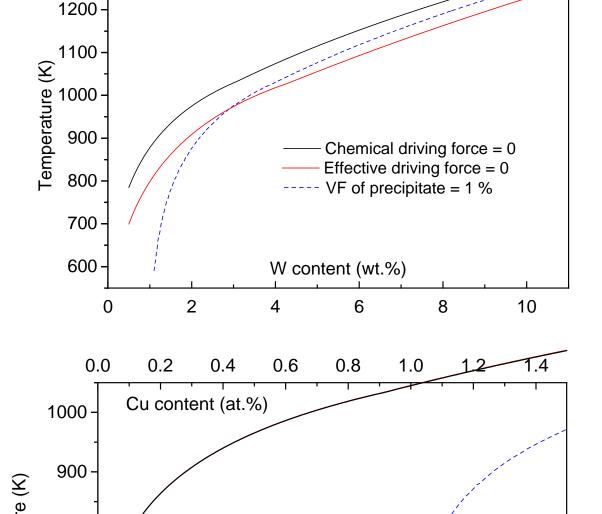
# **Model Description**



### Design of self-healing alloys

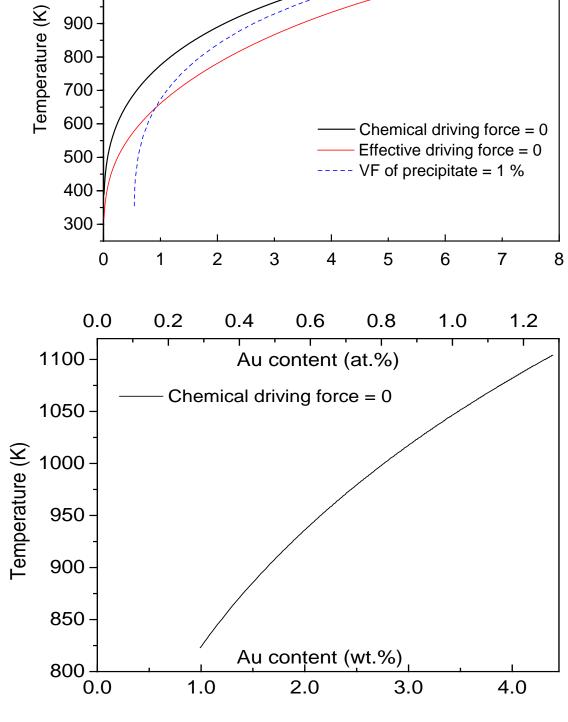
- Enough healing agent: volume fraction of precipitation phase > 1 %;
- Selectivity: precipitates form only on free surface





VF of precipitate = 1 %

1.5 2.0 2.5 3.0 3.5



1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5

- Cu: little shift of the solubility line due to minor volume misfit;
- Au: unlimited selectivity

800

Optimisation Module

- Precipitation strengthening: inversely proportional to the inter-particle spacing  $L^{[2]}$
- L increases during the coarsening of precipitates
- Aim for a small *L* and a low coarsening rate *K*.

$$r^{3} - r_{0}^{3} = Kt$$

$$L = r / \sqrt{f} = \sqrt[3]{r_{0}^{3} + Kt} / \sqrt{f}$$

$$K = \frac{8}{9} \frac{\gamma V_m^{\beta}}{\sum_{i=1}^{c} \frac{(x_i^{\beta} - x_i^{\alpha/\beta})^2}{x_i^{\alpha/\beta} D_i / RT}}$$

#### Design for creep resistance

- High strength martensite matrix
- Limited undesirable phases
- Corrosion resistance
- $M_S > 250 \, {\rm °C}$
- Adequate molar fraction of matrix phase
- Cr content > 8 wt.% in the matrix
- Parameters can be calculated by Thermo-Calc

#### **Future Work**

- To determine the optimal composition for the first generation creep resistant steel with the self-healing capability;
- The study of the creep behaviour of the designed alloy; the research on the mechanism properties after the healing behaviour;
- Model development and optimisation: the change in the driving force for precipitation during the healing process.

#### References

[1] S. Zhang, C. Kwakernaak, W.G. Sloof, E. Brück, S. van der Zwaag, N.H. van Dijk, Adv. Eng. Mater., 17 (2015) 598-603. [2] Q. Lu, W. Xu, S. van der Zwaag, Philos. Mag., 93 (2013) 3391-3412.

